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A Review on Particle Swarm Optimization variants and their applications to Multiple Sequence Alignment

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Abstract

Multiple sequence alignment is one of the most widely used techniques in bioinformatics for discovering functional, structural, and evolutionary information of biological sequences. Multiple sequence alignment is NP-complete problem and a challenging area of bioinformatics. Classical approaches are not efficient for such type of problem because of the increased time and space complexities. Hence, enormous metaheuristic are being applied in this field. Particle swarm optimization is one of the best developed and popular metaheuristics employed for various application domains. This paper discusses the Particle swarm optimization variants and their applications for multiple sequence alignment.

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1 Introduction

Bioinformatics is an application of computer technology for the analysis and management of biological and medicinal data. It includes creation and advancement of complex and large database and interfaces, development of algorithms and computationally intensive techniques for simulation and modelling of the biological process. Multiple sequence alignment (MSA) is one of the most substantial techniques in the sequence comparison. Sequence alignment searches for the conserved regions to find evolutionary relationship between species and the ancestors. Conserved sub-regions may represent important functions or regulatory elements. MSA is imperative for structure prediction, phylogeny, modeling binding sites, function prediction and many bioinformatics applications (*Das et al*. [15], *Durbin et al*. [19]).

Use of laboratory experiments and equipments for sequence alignment appears much time consuming, sensitive to experimental errors and expensive. Hence, a lot of computational efforts are being made from last two decades to develop efficient software tools to simulate the aligning process and an efficient model for accurate alignment of lengthy complex sequences at lesser time and space complexity. The methods to solve MSAs are divided into four distinct categories: Exact approach; Progressive approach; Consistency based approach; Iterative approach (*Notredame* [59]). The Exact approach dynamic programming (DP) was initially used for the pairwise alignment (*Needleman and Wunsch* [57]). DP searches the shortest path in a weighted direct acyclic graph so as to obtain the best alignment. It uses previous solutions of optimal alignment from smaller sub-sequences to build up the best possible alignment. DP fails quickly as the length and the number of sequences increases. Hence, DP is not feasible when $k \geq 4$ (*Lipman et al*. [43], *Carillo and Lipman* [6]). The Progressive approach contains less complexity in time and space (*Taylor* [76], *Feng and Doolittle* [22]). The alignment is constructed by starting with the most similar sequences and then incrementally aligning more distant sequences or groups of sequences to the initial alignment. The standard representative of progressive methods is CLUSTALW (*Thompson et al.* [77]). Other progressive algorithms include MUSCLE (*Edgar* [21]), MATCH-BOX (*Depiereux and Feytmans* [16]), MultAlign (*Corpet* [13]) and PileUp (*Devereux et al*. [17]). The main problem with progressive algorithms is: the dependence upon initial pairwise alignments and the choice of a suitable alignment scoring scheme. Consistency based approaches assume maximal consensus as the criteria of optimal alignment (*Kececioglu* [31]). Consistency based approaches include MWTP (maximum weight trace problem), T-COFFEE (tree-based consistency objective function for alignment evaluation) (*Notredame et al*. [61]; *Notredame et al*. [60]) and DIALIGN (*Morgenstern* [53]; *Morgenstern et al*. [54]; *Morgenstern and Werner* [55]; *Subramanian and Weyer - Menkhoff* [71]). When T-COFFEE is optimized by SAGA (sequence alignment by genetic algorithm), MSAs are solved by following MWTP. These methods have been shown to outperform most current MSA packages with regard to accuracy. But the cost for accuracy is a high time complexity in the order of O (k^3n^2), where k is the number of sequences and n is the length of longest sequence. An iterative algorithm starts with a generated initial alignment and iteratively refines it until no more improvement can be obtained. Hence the result does not depend on the initial pairwise alignment. The main objective of the iterative approach for MSA is to globally enhance the quality of a sequence alignment. These approaches include hidden Markov model (HMM) training (*Eddy* [20]; *Lytynoja and Milinkovitch* [48]; *Rasmussen and Krink* [65]), Gibbs sampling (for local alignment only) (*Lawrence et al*. [36]), simulated annealing (SA) (*Kim et al*. [33]), ant colony optimization (ACO) (*Chen et al*. [10]; *Moss and Johnson* [56]), and particle swarm optimization (PSO). Unfortunately, iterative algorithms lack speed and reliability.

Swarm intelligence (SI) is an emerging area of optimization, inspired by the decentralized way of working of swarms of social insects, flocks of birds or schools of fish. This behavior of swarms is mimicked and employed in artificial intelligence (*Blum and Li* [5]). A family of nature inspired algorithms has come into existence from last decade. The example of these swarm intelligence based techniques are Ant colony optimization, PSO, Artificial bee colony algorithm, Cuckoo search, Firefly algorithm, Multi-swarm optimization, Stochastic diffusion search, Gravitational search algorithm, Altruism algorithm, Artificial immune systems, Charged system search, Intelligent water drops, River formation dynamics, Self-propelled particles and many more [75]. SI based algorithm are found to be flexible and robust; hence nowadays it's taking the place of traditional algorithms for the complex, specifically the NP-problems.

As per the citation index PSO is the most popular SI based technique. PSO has high global convergence performance; requires primitive mathematical operators and a very few parameters to adjust; needs reduced memory and performs at an improved computation speed. These are the main reasons of PSO to be popular. Previous testing found the implementation of PSO to be effective with several kinds of problems and a lot of applications in various disciples, including bioinformatics. Applying PSO for MSA belongs to the fourth sequence alignment approach.

PSO too has a few drawbacks alike the other evolutionary algorithms (EAs), such as premature convergence, small search area and trapping in local optima. Many modified PSO algorithms have been proposed to overcome these drawbacks of PSO. More than 200 PSO variants have been developed till date. This paper discusses the most recent PSO variants and their applications in MSA. Section 2 presents the brief introduction of PSO algorithm followed by PSO variants till date in section 3. Section 4 gives the overview of all the MSA papers based on the PSO algorithms and variants. The paper is concluded in section 5.

2 Particle Swarm Optimization algorithm

PSO is a class of derivative-free, population-based computational methods for global optimization which is inspired by social behavior of bird flocking or fish schooling and derived by *Kennedy and Eberhart* in 1995 [32]. The particles (potential solutions) fly through the problem space by following the current optimum particles. Each particle keeps on tracking of its coordinates in the problem space which are associated with the best solution it has achieved so far, known as personal best. Another best value is the global best value, tracked by the particle swarm optimizer in the topological neighbors of all population (Yuan et al. [94]). Three characteristics are maintained by each particle as shown in equations (1-3):

1. The current position, x_i in search space. The position at time step *t* of a particle is updated by adding a velocity to its current position as follows:
$$x_i(t+1) = x_i(t) + v_i(t+1) \tag{1}$$
2. A personal best position, y_i is the best position that the particle has recorded since the first time step. When dealing with minimization, y_i at next time step *t* + 1 is computed as:
$$y_i(t+1) = \begin{cases} y_i(t), & \text{if} \quad f(x_i(t+1)) \geq f(y_i(t)) \\ x_i(t+1), & \text{if} \quad f(x_i(t+1)) < f(y_i(t)) \end{cases} \tag{2}$$
3. Its current velocity, v_i at time step *t*, the velocity $v_{i,j}(t)$ in dimension j is updated using:

$$v_{i,j}(t+1) = v_{i,j}(t) + c_1 r_{1,j(t)}[v_{i,j}(t) - x_{i,j}(t)] + c_2 r_{2,j}(t)[y'_{i,j}(t) - x_{i,j}(t)] \tag{3}$$

where c_1 and c_2 are positive acceleration coefficients regarding cognitive and social components respectively, while $r_{1,j}(t)$, $r_{2,j}(t) \sim U(0, 1)$ are uniform random numbers in the range [0,1]. The symbol $y'_{i,j}(t)$ refers to the neighborhood's best particle position vector so far. Pseudo code of the general PSO is given in figure 1. In a PSO algorithm, initialization is performed using random numbers and then fitness is computed for each particle. Then a loop starts to converge to an optimum solution. The loop is terminated with a stopping criterion predetermined in advance.

```
Initialize parameters
Initialize population
Evaluate
Do {
Find particle best
Find global best
Update velocity
Update position
Evaluate
} While (Termination)
```

Figure 1: General PSO Algorithm

3 Particle Swarm Optimization Variants

Due to the enormous applications of PSO, abundant literature is available on the variants of PSO. *Sedighizadeh and Masehian* [67] discussed all the major PSO variants till the end of 2008. The number of variants discussed was 95. This paper discusses the further variants since 2009.

Zhang and Sun [99] presented alternate two phases PSO (ATPPSO), including two processes, attractive and repulsive process. In the attractive process, each particle is attracted to its personal best position and the current global best position. Each particle is repelled away from its personal worst position in the repulsive process to increase the swarm diversity and speed up the convergence of the proposed algorithm. These two processes execute alternatively. Besides this, a fast makespan computation method based on matrix was designed to improve the algorithm speed. *Zhang et al*. [100] hybridized PSO with tabu search (TS) algorithm (PSO+TS) to solve the multi-objective flexible job-shop scheduling problem (FJSP) with many conflicting and incommensurable objectives. In PSO+TS approach, PSO assigns operations on machines and schedules operations on each machine, and TS performs local search for the scheduling sub-problem arising from each obtained solution. Proposed strategy was comparatively effective than other tested approaches. *Pant et al*. [63] introduced the sobol mutation variant for quantum inspired PSO (SOM-QPSO), based on the uncertainty principle that the position and velocity of the particle cannot be determined simultaneously. The concept of mutation was included in the QPSO, with SOM. SOM uses quasi random (sobol) sequence because these sequences cover the search domain more evenly than the random probability distributions, enhancing the chances of finding a better solution. Two versions of algorithms called SOM-QPSO1 and SOM-QPSO2 were defined based on the mutation of best and worst particle respectively. The significant improvement in performance of QPSO was found when applied with SOM operator. *Yuan et al*. [93] improved binary PSO (BPSO) method to solve the unit commitment problem (UCP), by integrated BPSO with lambda-iteration method and proposed improved BPSO (IBPSO). IBPSO is enhanced by priority list based on the unit characteristics and heuristic search strategies to repair the spinning reserve and minimum up-down time constraints. In proposed approach, BPSO solves the unit-scheduling problem and lambda-iteration method solves the economic load dispatch problem. BPSO and lambda-iteration methods run in parallel, adjusting their solutions for a better solution to solve UCP. *Wang et al*. [79] presented a two stage composite PSO (TS-CPSO) with the strategy of gradual range contraction. The strategy of TS-CPSO algorithm was divided into two phases. Firstly, a satisfactory solution group is searched, which is a rough extreme judgment. Secondly, based on the satisfactory solution groups derived in the first stage, the range of the optimization under a certain strategy is narrowed, in order to search for a global optimal or satisfactory solution. The simulation results showed that TS-CPSO had a good convergence performance under a rough extreme reservation strategy, especially for large-scale and high-precision optimization problems. *Li et al*. [40] proposed a heuristic particle swarm optimizer (HPSO) algorithm, which is based on standard particle swarm optimizer and the harmony search (HS) scheme. This algorithm is designed for discrete valued structural optimization problems. The testing results of five truss structure optimization problems showed that the HPSO algorithm had better global and local search behavior, was able to accelerate the convergence rate effectively. The comparison results showed that HPSO had the fastest convergence rate than PSO and the PSO with passive congregation (PSOPC) algorithms. *Moraglio and Togelius* [52] extended geometric PSO (GPSO) as inertial GPSO (IGPSO), by adding inertia term that applies to generic search spaces via a geometric interpretation of the dynamic of the particles governed by the full PSO equation. The construction of a weighted extension ray in Hamming space was described. Initial results of applying IGPSO to a classic benchmark were found promising. *Maeda et al*. [49] presented a combination of the PSO and the simultaneous perturbation optimization method as simultaneous perturbation PSO. The proposed method utilized local information of an objective function and global shape of the function. The results showed that the combinations of the global search capability of the PSO and the local search by one of the gradient method by simultaneous perturbation to be a promising approach. *Arumugam et al*. [3] dealt with extrapolation technique with PSO (ePSO). In ePSO the current particle position is updated by extrapolating the global best particle position and the current particle positions in the search space for updation of pbest and gbest.

The algorithm was applied to a real time application of steel annealing processing. The results showed that the proposed algorithm achieves the near global solution with faster convergence rate. *Alatas et al*. [1] presented a method that uses chaotic maps for parameter adaptation. The sequences generated from different chaotic systems substituted random numbers for different parameters of PSO where it was necessary to make a random-based choice. The proposed methods improved the global searching capability by escaping the local solutions and increasing the solution quality. *Alatas and Akin* [2] introduced fusion of chaos and PSO research field and presented chaotically encoded PSO algorithm (CENPSOA) that uses chaos decision variables and chaos particles based on the notion of chaos numbers. Chaos numbers generation was proposed in author's previous paper. A mathematical approach had been developed in this work that deals with chaos numbers and includes various chaos arithmetic and evaluation measures. *Zhou and Tan* [106] dealt with graphic processing unit-based parallel standard PSO (GPU-SPSO) to run PSO on GPU in parallel, based on compute unified device architecture (CUDA). GPU-SPSO was found to be capable to enlarge the swarm population and problem dimension sizes, speed up its running greatly and provide users with a feasible solution for complex optimizing problems in reasonable time. The running time of the SPSO based on GPU (GPU-SPSO) was found to be greatly shortened compared to that of the SPSO on CPU (CPU-SPSO). *Cui and Cai* [14] proposed integral-controlled PSO with dispersed accelerator information (IPSO-DAI) so as to improve the computational efficiency by employing a predefined predicted velocity index to guide the moving direction of particle. In proposed approach, if the average velocity of one particle is greater than the index value, it will have a convergent manner, else a divergent manner. Each particle’s performance to fit different living experiences decides the choice of convergent or divergent manner of the particle. Simulation results for IPSO-DAI showed that IPSO-DAI may provide a better performance when used for solving multi-modal functions compared with other three PSO variants. *Cervantes et al*. [7] dealt with Michigan approach PSO (MPSO) for prototype reduction in classification problems. MPSO approach has each particle in a swarm representing a single prototype in the solution and uses modified movement rules with particle competition and cooperation that ensures particle diversity. This work used nearest neighbor (NN) classification. Michigan approach used the binary version of PSO to discover a set of induction rules for discrete classification problems. As the result showed MPSO was able to reach better solutions in a much lower number of rule evaluations. *Mo et al*. [51] proposed conjugate direction PSO (CDPSO) for high-dimensional optimization problems. Conjugate direction method provides initial guess to optimize the problem so as to overcome the trapping in local minima problem by changing high-dimension function optimization problem into low-dimensional function optimization problem. PSO then efficiently solves the low-dimension function optimization problem. The numerical outputs showed that CDPSO successfully solved systems of nonlinear equations. *Lin and Chen* [42] dealt with PSO with linear discriminant analysis (LDA) to specify the beneficial features and to enhance the classification accuracy rate of LDA. This study showed that the classification accuracy rates of the PSOLDA were higher than many heuristic approaches, such as forward feature selection, backward feature selection, and PCA-based feature selection in many public data sets. *Kiranyaz et al*. [34] introduced multi-dimensional PSO (MD PSO) technique for the automatic design of artificial neural networks (ANNs). MD PSO was claimed to be capable to obtain the positional optimum in error space and also the dimensional optimum in the architecture space, even after the proper encoding of the network configurations and parameters into particles, because of no need of setting a fixed dimension a priori in PSO. A unique ANN configuration is obtained when the optimum dimension is converged at the end of a MD PSO process. The experimental results showed that the MD PSO generally evolves to optimum or near-optimum networks and had a superior generalization capability. *Oca et al*. [62] dealt with an algorithm that combines a number of algorithmic components of PSO variants that showed distinct advantages in the experimental study concerning optimization speed and reliability. This PSO variant known as Frankenstein's PSO was an attempt to gain insight into the performance advantages of different PSO algorithmic components and in improving understanding of the interactions among PSO variants.

Xinchao [84] proposed perturbed particle swarm algorithm (pPSA) with particle updating strategy based on the concept of possibility to deal with the problem of maintaining diversity within the swarm and to promote exploration in the search. The meaning of gbest in pPSA is "possibly at gbest (p-gbest)" instead of a crisp location in the fuzzy approaches. Experiments outputs indicated this approach to be effective in avoiding the local optimality with a non-increasing uncertainty. *Xie et al*. [83] presented amelioration PSO (SARPSO) based on SA, asynchronously changed learning genes (ACLG) and roulette strategy so as to escape from local optima. SA applied probability mutation in the search process so as to avoid the search processes of PSO plunging into local minimums; ACLG improved the ability of global search at the beginning, and was found to be promising to be convergent to global optimization in the end; the roulette strategy avoided the prematurely of algorithm. *Jin and Rahmat-Samii* [27] discussed hybrid real-binary PSO (HPSO) algorithm with its application in engineering electromagnetic, by evolving the real and binary variables in a hybridized vector simultaneously. Simulation and measurement results of optimized designs of three problems (i.e. a non-uniform antenna array, multilayered planar radar absorbing material and a dual-band handset antenna) found HPSO effective in obtaining designs with a high-quality performance. CPSOM is culture-based PSO with mutation (*Wu et al*. [82]). This algorithm is a fusion of cultural algorithm and mutation operator in PSO. CPSOM deals with improvement in the overall optimization performance and the premature problem of the original PSO. The mutation operator was applied to a proportion of the particles in the population space based on the influence function and was directed by the knowledge stored in the belief space. CPSOM deals with improvement in the overall optimization performance and the premature problem of the original PSO. *Zhang et al*. [102] introduced circular discrete PSO algorithm (CDPSO) for solving the flow shop scheduling problem. Particle similarity and swarm activity metric were defined in this algorithm. CDPSO contains an order strategy to preserve the diversity of the swarm. If the adjacent particles' similarity is greater than its current similarity threshold, the mutation operator mutates the inferior. CDPSO algorithm performance results were claimed to be greatly better than the compared GA and similar PSO algorithm (SPSOA) and acquiring the best convergence property.

Kiranyaz et al. [35] extended the idea of author's previous paper by introducing fractional global best formation (FGBF) technique for yielding a robust solution, specifically for multimodal complex problems at high dimensions. The proposed technique collects all the best dimensional components and fractionally creates an artificial global best (αGB) particle which has the potential to be a better "guide" than the PSO's native gbest particle. In this way, the potential diversity existing among the dimensions of swarm particles can be efficiently used within the αGB particle. *Venter and Haftka* [78] presented constrained PSO by a specialized bi-objective PSO algorithm. This algorithm uses a pareto based multi-objective PSO approach to solve the resulting bi-objective optimization problem. The constrained optimization problem is first converted to a bi-objective problem. A multi-objective PSO algorithm is then used to solve the resulting multi-objective optimization problem. This algorithm works particularly well for optimization problems with inequality constraints. As per the results, proposed algorithm's performance was competitive to that obtained from a penalty function implementation, with the benefit that no tuning of the constraint handling logic is required. *Song et al*. [69] proposed PSO algorithm based on predatory search strategy (PS-CPSO). They dealt with the centroid of particle swarm in the standard PSO model and adaptive space mutation to improve global optimum efficiency, speed and accuracy of algorithm. Simulation results showed that PS-CPSO improves the local searching efficiency and global searching performance greatly. The algorithm had faster convergence speed, higher precision and was able to effectively avoid the premature convergence problem. *Zhang et al*. [98] proposed a hybrid alternate two phases PSO algorithm (ATPPSO) for the flow shop scheduling problem which combined PSO with the genetic crossover operators, and annealing strategy. Each particle contained the attractive state and the repulsive state. The shortcoming of premature convergence was abstained in ATPPSO. A two point reversal crossover operator was constructed and in the repulsive process each particle was repelled away from some inferior solution in the current tabu list to fly towards some promising areas.

Sun et al. [73] presented modified PSO (MPSO) for optimization of mixed-variable problems. The average velocity of the swarm was proposed as a disturbance to expand the search range for each particle, to overcome the premature convergence. The value of different kinds of variables was proposed to be achieved according to their respective flying velocities. Experimental results showed that MPSO is simple, generic, easy-to-implement and highly competitive compared with existing algorithms. *Wu* [81] introduced embedded chaotic PSO (ECPSO) that uses chaotic mappings for parameter adaptation of wavelet v-support vector machine (Wv-SVM). ECPSO was consisting two PSO with adaptive and normal gauss mutation operators (ANPSO) existing in father process and child process respectively. The local optimal particle is obtained from child process and the global optimal particle is obtained from father process. ECPSO introduced chaotic mappings with ergodicity, irregularity and the stochastic property into ANPSO to improve the global convergence by escaping the local solutions. *Chuang et al*. [11] presented Chaotic catfish PSO (C-CatfishPSO) introducing chaotic maps into CatfishPSO, which increase the search capability of CatfishPSO via the chaos approach. Catfish particles replace particles with the worst fitness and initialize a new search from extreme points of the search space when the gbest fitness value is not changing from a certain number of consecutive runs. In this approach the logistic map was introduced to improve the search behavior and to prevent the particles being trapped in a locally optimal solution. Statistical analysis of the experimental results showed the superiority of C-CatfishPSO over PSO, C-PSO, CatfishPSO, and few other advanced PSO methods.

Chen et al. [9] presented inertia weight PSO (IWPSO) algorithm with Boltzmann exploration to adaptively tune the weights of individual and social cognition terms in velocity update equation so as to balance the exploration and exploitation in search process. IWPSO with Boltzmann exploration was claimed to be capable to guide particle for searching the promising region, hence has high effective searching capability. *Cooren et al*. [12] presented MO-TRIBES (multi-objective TRIBES), where TRIBES is a parameter free variant of PSO. MO-TRIBES is an adaptive Multiobjective PSO algorithm. The structure of the swarm and strategies of displacement of the particles were modified during the process according to the behavior of tribes. Pareto dominance criterion was the deciding factor for the final solution. To maintain the diversity along the Pareto Front the rules based on crowding distance were incorporated in the algorithm. The algorithm has multiple restarts so as to maintain the diversity. MO-TRIBES gave better results than other competitive algorithms NSGA-II and MOPSO. *Chen* [8] proposed a two-layer PSO (TLPSO) with a structure of two layers (top layer and bottom layer) which contains M swarms of particles generated in the bottom layer and one swarm of particles generated in the top layer. The global best position in each swarm of the bottom layer is set to be the position of the particle in the swarm of the top layer. Besides, a mutation operation was added into the particles of each swarm in the bottom layer which makes the particles leap the local optimum to find the global optimum. The simulation results for nine benchmark functions showed that TLPSO performed better than the other compared EAs in the ability of finding the global optimum solution. *Ran and Si-qing* [64] proposed improved PSO algorithm (IPSO) for optimal reactive power dispatch and voltage control of power system.

A discrete PSO (DPSO) algorithm was introduced to construct the collection of discrete values, so as to let the whole optimization process more accurately reflect the real power system operation. The adaptive parameters of strategies are utilized to make the performance of PSO algorithm more effective. IEEE 30-bus power system was evaluated using IPSO algorithm. The results showed that IPSO had better global search ability and the fast searching speed. *Shi et al*. [68] hybridized cellular automata (CA) and PSO as cellular PSO (CPSO) for function optimization. CPSO contains a mechanism of CA integrated in the velocity update of PSO to modify the trajectories of particles to avoid stagnation. With CA and PSO are integrated in two different ways and form two versions of CPSO, i.e. CPSO-inner and CPSO-outer. The CPSO-inner uses the information inside the particle swam to interact by considering every particle as a cell. The CPSO-outer enables cells that belong to the particle swarm to communicate with cells outside the particle swarm with every potential solution defined as a cell and every particle of the swarm defined as a smart-cell. The experimental results showed that the proposed method was performing better than the other tested variants of PSO on benchmark test functions. *Mei et al*. [50] proposed PSO algorithm based on a periodic evolution strategy (PSO-PES) on the concept of updating of the best solution by a periodic evolution strategy. This work is based on the idea of controlling the energy of particles. A perturbation strategy was designed to construct a dissipative system of particles. A size limit function was proposed to control perturbations, which was based on particles' energy. *Li et al*. [38] presented recursive PSO (R-PSO) algorithm, which searches the solution space recursively according to the one by one coming data and adjust their steps dynamically according to search space size and the fitness of each particle itself during the optimization process. R-PSO did well in improving the cognitive ability of individuals to adapt to new datum constantly. The performance of radial basis function network modeling system based on R-PSO was poor while there wasn't enough learning data but it showed betterment along with the increase of learning time. *Yen et al*. [92] dealt with modified hybrid PSO (MHPSO), determined by a combination of modified real PSO and modified binary PSO to improve their performance. PSO was coupled with the proposed heuristic based constraint satisfaction approach to make the solutions feasible for PSO. The velocity equation of particle was revised to prevent particle stagnation. Unit commitment priority was used to improve the performance of binary PSO. *Yang and Jin* [90] proposed hierarchy PSO (HPSO) algorithm for solving a multi-objective daily generation scheduling model for the hydropower stations. The model contains two objective functions including maximization of peak-energy capacity benefits and maximization of power generation. In this algorithm an accelerating genetic operator based on the characteristics of peaking operation of hydropower stations was designed, which remarkably improved the convergence performance and search efficiency of HPSO. *Yang et al*. [91] used a combination of Accelerated PSO and a nonlinear support vector machine to form a structure for solving business related optimization problems. The proposed approach PSO-SVM was applied to three case studies production optimization, income prediction and project scheduling. *Sun et al*. [72] dealt with double PSO (DPSO), based on modified PSO (MPSO) as a global search algorithm and PSO with feasibility-based rules do local searching. The variant was developed for the best consistent optimal results for mixed-variable optimization problems. Feasibility-based rules were used as the handling mechanism for constraint conflict. DPSO uses MPSO for non-continuous variables' valuing, and the fast convergence of PSO for finding the continuous optimization problems. The simulation results of DPSO for two real-world mixed-variable optimization problems were found to be highly competitive compared with other existing algorithms.

Zhang et al. [103] proposed a two-stage PSO (PSO) algorithm for stochastic job shop scheduling problem (SJSSP) with the objective of minimizing the expected total weighted tardiness. JSSP is strongly NP-hard. Firstly, a performance estimate was used for quick evaluation of the solutions, and a local search procedure was embedded for accelerating the convergence for promising regions in the solution space. Then PSO started the search process, by applying Monte Carlo simulation. For reducing the computational burden, the optimal computing budget allocation method was used. *Liang et al*. [41] dealt with an existing fitness euclidean-distance ratio PSO (FER-PSO) proposing memetic FER-PSO. A local search method was introduced and combined with FER-PSO to improve its fine search ability or the ability to identify multiple optima. Proposed niching algorithm was found to outperform its original version and many other niching algorithms. *Zhang and Wu* [105] proposed a hybrid restarted simulated annealing PSO (RSAPSO) technique to find global minima efficiently and robustly. RSAPSO is the combination of local search ability of RSA and global search ability of PSO. *Zhang et al*. [104] proposed elite quantum behaved PSO (EQPSO) algorithm employing elite strategy for the global best particle to prevent premature convergence of the swarm. They applied this algorithm to solve bi-level multi-objective programming problem. *Wei et al*. [80] employed local stable mechanism in PSO and proposed improved PSO (IPSO). IPSO takes a specific population zone at a stable level and the remaining zone uses harmony search. The algorithm was found to be effective in avoiding the premature convergence and improving the ability of searching optimum solution with increased convergence speed. *Xia et al*. [85] proposed multi-swarms competitive PSO (MSCPSO) based on fuzzy C means clustering. Out of two scale swarms, large scale swarms use standard PSO and small scale swarms randomly search in the optimal solution neighborhood. This technique improves the possibility of jumping out from local optima and increases the diversity of the swarms. Inspired by Artificial Bee Colony algorithm (ABC), ABC-PSO algorithm was proposed by *Hu et al*. [24] to ensure for PSO not to get trapped in local optima. After employing PSO all the particles get into the new position and then ABC mechanism is applied on the concept of evaluation and selection. *Noel* [58] presented gradient-based PSO (GPSO) algorithm. GPSO doesn't need inertial weights and constriction coefficients and is claimed to achieve faster convergence and better accuracy. *Xu et al*. [87] simulated the population size of the human evolution for PSO with increment of particle size (IPPSO). Proposed algorithm was found to be performing better at time and efficiency for logistic model than linear function for complex problems. *Dor et al*. [18] presented a multi Swarm PSO algorithm DEPSO-2S, which is a hybridization of DE and PSO. DE constructs only those swarms that gather the best particles of auxiliary ones. *Bhattacharya et al*. [4] introduced a family of position mutated hierarchical PSO algorithms with time varying acceleration coefficients (PM_nHPSO-TVAC where n = 1, 2, 3, 4). It doesn't have any controlling parameters. Because of position mutation schemes the swarms get out of local optima traps and because of the hierarchical nature of the swarm premature convergence is prevented. *Yu et al*. [96] PSO based on two sub swarms (TSS-PSO) having divided two identical sub-swarms. First sub-swarm based on basic PSO to evolve and second sub-swarm iterates adopt the cognition. The worst fitness of the first sub-swarm is replaced with the best fitness of the second sub-swarm in every iteration for enhancing the diversity and improving the convergence of the algorithm.

4 Particle Swarm Optimization for Multiple Sequence Alignment

Due to the simplicity and robustness of PSO algorithms, many developments have been performed in PSO to find the optimal alignment of NP-hard MSA problems, which are divided in two subsections i.e. MSA with direct application of PSO and MSA with training of HMM by PSO. Table 1 presents the overview of all PSO approaches applied for MSA along with the description of benchmarks and the PSO variants applied.

4.1 Direct application of PSO

Lv et al. [47] discussed an application of improved PSO applied for MSA to diagnose system for colonic cancer in pervasive environment. High quality MSA of Proteins was needed to be performed for correct decision making hence two improved EAs (GA and PSO) were applied for improving the performance of MSA. In improved GA the segment profiles were introduced to speed up the convergence. The principles of information diffusion and clone selection in improved PSO (IDCSPSO) were incorporated to prevent premature convergence problem. IDCSPSO gave best results on benchmarks with medium and high similarity but bad alignment on some low similarity benchmarks. In that specific problem it suited the best, because the protein sequences of patients were highly similar. *Rodriguez et al*. [66] used the alignment obtained from CLUSTALX as the initial alignment and then applied PSO. The approach named PSOAlign is based on the concept of improving the alignment obtained from CLUSTALX.

PAM250 matrix was used for the evaluation of the alignment. In PSOAlign every aligned sequence was taken as a coordinate, a distance measure between alignments was proposed and a movement mechanism for the particles as well. PSOAlign succeed in improving the alignments in most of the cases. In *Zablocki* [97], a detailed description had been provided for applying PSO for MSA. Two different search spaces were used for the study i.e. integer search space as default and binary search space as per requirement. A wide empirical analysis was done.

S8 analysis was performed to evaluate the influence of individual standard PSO (S-PSO) characteristics and binary PSO (B-PSO) characteristics on S8 data set, which is low complexity MSA dataset. Then the scalability analysis was conducted extending the empirical analysis for more complex data sets. S-PSO, mutating PSO (M-PSO) and cooperative split PSO (CPSO-SK) were compared, at the basis of their performance in aligning the sequences. When the velocity of S-PSO was initialized randomly with using similarity method, the alignment was superior. When the number of particles in a swarm was increased, the solutions improved. It was found that S-PSO was good for small alignment with high similarity. CPSO-SK was found to be offering more flexible solutions. *Juang and Su* [28] proposed a hybrid algorithm for MSA. The algorithm combined the pairwise dynamic programming (DP) and PSO to overcome computational and space complexity and local optimum related problems for MSA, when using DP.

Pairwise DP aligns sequences progressively and PSO works as an improver for a progressive pairwise DP by amending the alignment results to avoid being trapped into local optima. The approach was found to be promising and outperforming CLUSTALW for complex MSA problems. *Xiong et al*. [86] dealt with a method for MSA based on PSO with mutation operator, with the ability to improve local convergence. It was concluded that the improved algorithm was feasible and efficient. *Lei et al*. [37] used chaotic PSO for MSA to overcome the premature convergence problem effectively. When PSO appears for premature convergence, the chaotic search is used to update the particle of the current population by generating: chaotic variables between 0 and 1 when initializing the population so that the particles are distributed uniformly in the solution space; the chaotic sequences using the logistic mapping function so as to do chaotic search and strengthen the diversity of the population. The results showed that the proposed algorithm was found to be effective, can improve search performance for some sequences. *Xu and Chen* [89] proposed an improved PSO algorithm PSOMSA with three operators gaps deletion, gaps insertion, and local search operator. The performance of the algorithm was compared with CLUSTALX 2.0 and was found to be performing better. *Long et al*. [46] applied binary PSO (BPSO) for MSA. The alignment outputs were compared with CLUSTALW 1.83, T-Coffee 1.37, SAGA, and DIALIGN 2.2.1. Sum-of-pairs score (SPS) and column score (CS) were calculated for finding the alignment accuracy. Nine sequence sets were taken for the alignment and it was concluded that BPSO may perform well for short sequences, but were not found better on medium and large sequences. *Long et al*. [45] proposed mutation-based binary PSO (M-BPSO) for MSA. In the M-BPSO algorithm, BPSO algorithm was applied to provide alignments.

Thereafter, mutation operator was performed to move out of local optima and speed up convergence. MSA algorithm based on PSO with probability statistic and automatic adaptive mutation (MSA_PMPSO) was proposed in *Zhang et al*. [101]. MSA_PMPSO is based on a model, which works according to the distributional probability of high quality solutions. The algorithm introduced the fitness variance, the expected optimal solution and the mutation operation, so as to jump out of the local optima. The algorithm was concluded to be feasible, valid and suitable for the alignment of large-scale closed genetic long sequences. *Jagadamba et al*. [25] proposed MSAPSO based on optimizing the similarity score, residue match and execution time of the sequences aligned. For the sake of computation simplicity the matrix formed from the aligned sequences was restricted to an order of 2. Whole sequence was not taken at once to form a matrix of order equal to length of the sequence. The results were obtained at reduced time complexity. *Yu J* [95] improved the basic PSO algorithm for MSA by applying the concept of chaos optimization. This algorithm uses chaos searching to avoid local convergence and to enhance the ability of global convergence. The method was found suitable for medium and short length sequence of DNA and Protein.

A method of getting inertia weight and subsection weight (SW) was discussed in *Xu et al*. [88]. This paper dealt to solve local optima and slow convergence problems. At initial stages diversity of swarm was increased and at the later stages the convergence was accelerated. Experimental outputs showed that the early converging problem was avoided and the precision increased in solving MSA using this technique. *Kamal et al*. [30] applied parallel PSO for global MSA. Proposed parallel PSO was implemented using the massage-passing interface (MPI) library, tested over Linux cluster at EUMed Grid.

4.2 Training of HMM by PSO

Rasmussen and Krink [65] proposed a hybrid algorithm by combining PSO and EAs so as to train HMM to align sequences. It was the main emphasis of this paper to find an efficient method to train HMMs. The hybrid algorithm PSO-EA hybrid is different than PSO because of the breeding operation. The breeding process iterates through all particles and occasionally applies breeding to two particles with a specific probability. This approach was found to be better than SA and Baum-Welch methods for training HMMs.

Ge and Liang [23] proposed an immune PSO (IPSO), designed on the base of the models of vaccination and receptor editing in immune systems to train HMMs. Then an integration algorithm based on the HMM and IPSO was constructed. IPSO contains the randomness in stochastic optimization algorithms, hence is able to solve non linear optimization problems and acquired the adaptive ability that enables the algorithm to solve machine learning problems. The numerical outputs showed that the proposed algorithm produced the effective alignment and reduced the time cost. *Ji et al*. [26] proposed a HMM training method for multiple sequence alignment based on quantum-behaved PSO (QPSO) algorithm. This approach tried to overcome the limitations of Baum-Welch training HMM, by searching the feasible sampling space for the global optima. This algorithm claimed to improve the alignment abilities.

Long [44] presented diversity-controlled quantum-behaved PSO (DCQPSO). Firstly profile HMM was trained. Then, an algorithm was created for MSA, which was based on the integration of profile HMM and DCQPSO. The results showed that DCQPSO produced optimal alignments. *Li et al*. [39] presented an integration algorithm based on the profile HMM and QPSO for the MSA. Quantum-behaved

PSO (QPSO) was used to train profile HMM. The algorithm was claimed to be global convergent compared to its predecessor PSO algorithms and had only position vector, also it had fewer parameters to adjust than PSO. QPSO was found to be remarkably effective HMM training method. HMM trained by the QPSO, taking sum-of-pairs (SOP) as objective function, produced better alignment than all of the other compared methods. In *Sun et al.* [74] QPSO was mathematically analyzed. The analyses had been made for a single particle's behavior in QPSO, deriving the necessary and sufficient condition for probabilistic boundedness of the particle that guarantees the particle swarm to converge. Then an improved version diversity-maintained QPSO (DMQPSO) was proposed to maintain the diversity at a certain level to enhance the global search ability of QPSO. The averaged normalized scores DMQPSO-trained HMMs had the best average normalized scores, namely, the best overall performance in the tested MSA problems than ClustalW and the HMMs trained by BW, PSO and QPSO.

Table 1: Overview of PSO variants applied for MSA

Author	**PSO variant employed**	**Concept**	**Data set tested**	**Benchmark tested**
Rasmussen and Krink [65]	PSO-EA hybrid based on a breeding operation between position vectors using crossover operator	Training HMMs by using PSO-EA hybrid	Protein	Pfam database, BAliBASE
Ge and Liang [23]	Immune PSO (IPSO): Based on immune systems (Receptor Editing and Vaccination Model)	Introduced IPSO to train hidden Markov models (HMMs)	Protein	BAliBASE
Ji et al. [26]	Quantum-behaved PSO (QPSO) and QPSO with selection	Training HMMs by using QPSO and SQPSO	-	-

	operation			
Lv t al. [47]	PSO based on Information Diffusion and Clone Selection (IDCSPSO)	PSO and GA were applied to structurally align similar regions of multiple protein sequences of Colonic Cancer patients	Protein	BAliBASE3
Fabien B R Zablocki [97]	Binary PSO, Mutating PSO, Cooperative split PSO	Different combinations of neighborhood topologies, PSO parameters, MSA parameters, weightage, variants, scoring schemes, gap models were tested to obtain the optimal	DNA, RNA	EMBL
Rodriguez et al. [66]	No variant	Crossover operator applied to improve the ClustalX alignment	Protein	BAliBASE
Juang and Su [28]	Modified PSO proposed in Kennedy and Eberhart [32]	Combining pairwise DP and PSO to align sequences progressively	Protein	Clusters of orthologous groups (COGs)
Lei et al. [37]	Chaotic PSO (CPSO)	Generating chaotic variables at initialization and chaotic sequences using Logistic mapping function	Protein	BAliBASE
Long et al. [45]	Mutation-based Binary PSO (M-BPSO)	BPSO algorithm was applied to provide alignments, then mutation operator applied to move out of local optima and speed up convergence	DNA, Protein	-
Long et al. [46]	Binary PSO (BPSO)	Creating a binary matrix i.e. 0 for gap, 1 for alphabet	Protein	BALiBASE3
H X Long [44]	Diversity-controlled QPSO (DCQPSO)	Training profile HMMs by using DCQPSO	Nucle-otides	-

			and protein	
Zhang et al. [101]	PSO with probability statistic and automatic adaptive mutation (PMPSO)	Generation of new solutions with the help of a model on distributional probability of high quality solutions	Protein	BAliBASE
Xu and Chen [89]	Improved PSO with three operators: gaps deletion, gaps insertion, and local search operator	PSOMSA: removing only gap columns; inserting gap columns into the current best alignment; removing some gaps randomly from all the sequences to enhance the search performance	Protein	BAliBASE
Li et al. [39]	QPSO	Training profile HMMs by using QPSO	Protein	BAliBASE
Jagadamba et al. [25]	No variant	MSAPSO as an extension of PSAPSO based on creating 2x2 matrix of residues	Protein	Pfam database
Jian Yu [95]	Chaos PSO	Applied chaos searching to enhance global convergence	DNA, Protein	From Uniprot, NCBI
Kamal et al. [30]	Parallel PSO algorithm	Applied parallel programming to improve the ClustalX alignment as initial alignment	Protein	BAliBASE and SABmark
Sun et al. [74]	QPSO and Diversity-Maintained QPSO (DMQPSO)	Training profile HMMs by using QPSO and DMQPSO	Protein, DNA, RNA	Nucleotide sequences: generated Stoye et al. [70], Protein: Pfam and BALiBASE

5 Conclusion

This paper presents a review of Particle Swarm Optimization Variants developed till date and their applications to Multiple Sequence Alignment. The conclusion drawn after a wide research regarding the variants and their successive applications to MSA is that:

- PSO gives better results in terms of speed, accuracy, efficiency and robustness, if the local convergence problem, the tendency of getting trapped in local minima is removed and the global search ability is enhanced. For the same the hybridized PSO strategies with other efficient techniques gives significant betterment in the output.
- PSO algorithms with small modifications has got a lot of applications in multi-disciplines, including flow shop scheduling problem, engineering electromagnetic, business related optimization problems, unit commitment problem, optimal reactive power dispatch, voltage control of power system, automatic design of Artificial Neural Networks, multi-objective daily generation scheduling for hydropower stations and many bioinformatics problems including MSA.
- PSO is found to be quite efficient in solving MSA related problems. In earlier stages the trend was to train HMM using different approaches and then perform MSA. For improvement in HMM training approach many efforts were done. Then the inclination was in the direction of hybridization of PSO with efficient techniques, improvements in initial alignments, introducing operators, inclusion of concept of chaos, applying those PSO variant which are already proved to be efficient and recently the analysis of the PSO variants in order to improve them to make suitable for MSA.

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